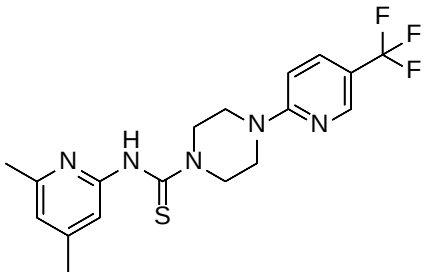
Product data sheet

MedKoo Cat#: 561459 Name: NCT-502 CAS: 1542213-00-2 Chemical Formula: $C_{18}H_{20}F_3N_5S$ Exact Mass: 395.1392 Molecular Weight: 395.4482	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
NCT-502 is an inhibitor of human 3-phosphoglycerate dehydrogenase (PHGDH). NCT-502 reduces the production of glucose-derived serine in cells and suppresses the growth of PHGDH-dependent cancer cells in culture and in orthotopic xenograft tumors.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	25.0	63.22
DMSO	70.0	177.01
Ethanol	1.0	2.53
Ethanol:PBS (pH 7.2) (1:10)	0.33	0.83

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.53 mL	12.64 mL	25.29 mL
5 mM	0.51 mL	2.53 mL	5.06 mL
10 mM	0.25 mL	1.26 mL	2.53 mL
50 mM	0.05 mL	0.25 mL	0.51 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Rohde JM, Brimacombe KR, Liu L, Pacold ME, Yasgar A, Cheff DM, Lee TD, Rai G, Baljinnyam B, Li Z, Simeonov A, Hall MD, Shen M, Sabatini DM, Boxer MB. Discovery and optimization of piperazine-1-thiourea-based human phosphoglycerate dehydrogenase inhibitors. Bioorg Med Chem. 2018 May 1;26(8):1727-1739. doi: 10.1016/j.bmc.2018.02.016. Epub 2018 Feb 27. PMID: 29555419; PMCID: PMC5891386.

In vivo study

1. Shen L, Zhang J, Zheng Z, Yang F, Liu S, Wu Y, Chen Y, Xu T, Mao S, Yan Y, Li W, Zhang W, Yao X. PHGDH Inhibits Ferroptosis and Promotes Malignant Progression by Upregulating SLC7A11 in Bladder Cancer. Int J Biol Sci. 2022 Aug 29;18(14):5459-5474. doi: 10.7150/ijbs.74546. PMID: 36147463; PMCID: PMC9461664.

7. Bioactivity
Biological target:

Product data sheet

NCT-502 is a human phosphoglycerate dehydrogenase (PHGDH) inhibitor, cytotoxic to PHGDH-dependent cancer cells, and reduces glucose-derived serine production, with an IC_{50} of 3.7 μM against PHGDH.

In vitro activity

As previously reported, NCT-502 (27) and NCT-503 (31) reduced the production of glucose-derived serine in cells and suppressed the growth of PHGDH-dependent cancer cells, both in culture and in orthotopic xenograft tumors. The metabolic effects of these molecules were found to be largely specific to PHGDH and downstream pathways linked to serine flux. However, NCT-502 (27) inhibitor treatment was found to reduce aspartate levels in cells, irrespective of PHGDH levels; decreased oxygen consumption was observed in the presence of both active and inactive representatives of this chemotype, suggesting the effect may be driven in part by electron transport chain inhibition.

Reference: Bioorg Med Chem. 2018 May 1;26(8):1727-1739. https://pubmed.ncbi.nlm.nih.gov/29555419/

In vivo activity

For this, NCT-502 or vehicle control (PBS) was injected intratumorally every three days after tumor injection, and then subcutaneous xenografts were peeled off after 4 weeks. The results showed that the xenografts in the NCT-502-injected mouse group were significantly smaller compared to those displayed by the vehicle group (Figure (Figure5B-D).5B-D).

Reference: Int J Biol Sci. 2022 Aug 29;18(14):5459-5474. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9461664/